

Extraordinary behavior of β -hydroxy sulfoxides and sulfone of pinane series

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Abstract

© 2017 Taylor & Francis Group, LLC. The “racemic compound-like” behavior, low-temperature conformational rearrangement and “crystallization-induced diastereomerization” of β -hydroxysulfoxides and sulfone of pinane series have been studied. It was established, that the sample of sulfoxide crystallizes as an asymmetric dimer containing a supramolecularcentrosymmetric moiety formed through $S=O\cdots H-O$ interactions between two independent molecules. Moreover, it was found that this dimer can crystallize in two so-called “packing polymorphs”—monoclinic and triclinic ones. By transition from the room temperature to 150 K for both polymorphic forms conformational restructuring of a stable hydrogen-bonded synthon from “unfolded” form to “folded” one has been observed. The sample of sulfoxide is interesting as the first example of the co-crystallization of chiral sulfur compounds. Surprisingly we have found a similar H-bonded dimer, formed by independent molecules, where all sulfone molecules are identical in stereochemical aspect. We suggested to use the new term “crystallization-induced diastereomerization” for the description of the stereochemical process leading to the formation of sulfone dimer. From a supramolecular chemistry point of view, we can speak of the finding of a new robust and reproducible synthon. From a stereochemical point of view, an “enantiphilic” fragment was discovered—a β -hydroxysulfoxide or sulfone group, capable of recognizing its mirror image.

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Keywords

(–)- β -pinene, crystallization-induced diastereomerization, polymorphic modifications, β -hydroxysulfone, β -Hydroxysulfoxide, “racemic compound-like” crystallization

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